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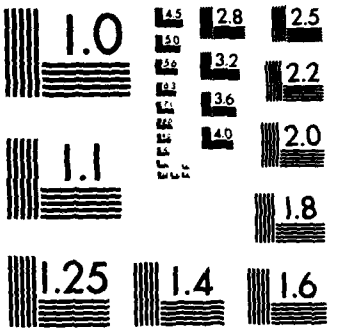

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SOLUTION METHODS FOR LARGE SPARSE LINEAR SYSTEMS

Final Technical Report

by

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The discretisation of partial differential equations, by either finite element or finite difference techniques, often leads to large linear systems of equations with sparse matrices. Fast iterative solution methods, based upon the preconditioning of the conjugate gradients method, have been proposed for the symmetric positive definite case [11] and also for more general situations. ~~in [12]~~ In this report we present new sharp upperbounds for the conjugate gradients residual. These upperbounds help us to understand and explain the convergence

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cont → behaviour of the preconditioned conjugate gradients method. We also present a type of preconditioning that has almost the same convergence properties as those presented, ~~in [1]~~ but which admit- full vectorization on supercomputers like the CRAY-1 and the CYBER 205.

For the nonsymmetric case we propose different types of preconditioning in connection with the Chebyshev iterative method.

1. INTRODUCTION

The aims of the research, as carried out during the years of the contracting period, have been threefold:

1. To explain the speed of convergence of the preconditioned conjugate gradients method (for the symmetric positive definite case).
2. To construct fast iterative methods for sparse linear systems with nonsymmetric matrices.
3. To develop user-oriented software for the methods mentioned in the previous two points.

As may appear from section 2 and 3, considerable progress has been made with respect to all the above listed points. The results which have been obtained have all been published recently or they have been submitted for publication. Major part of the research has also been published in the form of a Ph.D.-thesis [3].

In section 2 we present an overview of the results obtained for the symmetric positive definite case and in section 3 we introduce the results for the nonsymmetric case.

2. SYMMETRIC POSITIVE DEFINITE MATRICES

In this case we consider the conjugate gradients (cg) method for the iterative solution of $K^{-1}Ax = K^{-1}b$, where $Ax = b$ is the linear system to be solved and K^{-1} is a preconditioning matrix. For a description of this method see [1].

In [3, chapter 2] an analysis of the convergence behaviour of the cg method is presented, which exploits its relationship to the Lanczos method. This analysis leads to an expression for the residual in terms of the Ritz values (i.e. the eigenvalue approximations generated by the Lanczos method).

It has been observed, e.g., by Concus et al. [4], that in many relevant situations the convergence behaviour appears to be much better than might be expected from upperbounds involving only the condition number of $K^{-1}A$. This so-called superlinear convergence behaviour can, even for rather dense spectra, be fairly well explained by our upperbounds (see [3, chapter 2]), which take advantage of the relative separation of the smallest eigenvalues.

For a specific example of the preconditioned method it is shown that the separation of only the four smallest eigenvalues is sufficient to explain the actual

observed convergence behaviour. This contrasts with the widespread belief that it is the clustering of the eigenvalues that causes the fast convergence.

It is one of the purposes of [3, chapter 3] to show that for a class of model problems (i.e., the discretised Poisson equation) the preconditioning of A should always give a more favourable eigenvalue distribution, in particular with respect to the smallest eigenvalues.

In view of the dependence of the convergence behaviour of cg upon the separation of the smallest eigenvalues of the operator, we also comment in [3, chapter 3] on certain modifications of the ICCG method, which have been proposed in litterature (e.g., see [5]).

In [2] a family of incomplete decompositions is presented, to be used as preconditioning matrices for the cg method. The question which member of this family leads to optimal results (with respect to efficiency) remains unanswered. However, the results of numerical experiments given in [2], may help in the choice.

For the simplest types of incomplete decomposition Eisenstat [6] has shown that the preconditioned cg algorithm can be implemented in such a way that the number of arithmetical operations per iteration is almost the same as for the unpreconditioned cg algorithm. This makes the use of these decompositions even more attractive.

The use of incomplete decompositions on vector computers gave some problems, since they do not automatically lead to vectorizable algorithms [7,8]. Only with the help of laborious permutations the efficiency of this algorithm, as compared with other algorithms, can be restored [8,9]. In [10,11] a simple variant of the incomplete decomposition algorithm is introduced which admits full vectorization without notable loss in the number of iterations and instability.

Software for the preconditioned cg algorithm is available in the program library ACCULIB [12,13].

Remark. For the actual computation of the extreme eigenvalues of the preconditioned operator we have used a generalized Lanczos scheme. This scheme has been developed as a side-product of the research and has been described in [14].

3. NONSYMMETRIC MATRICES

Here we consider the use of the complex Chebyshev Iteration method for the solution of $K^{-1}Ax = K^{-1}b$, where K^{-1} is a suitable preconditioning matrix for the linear system $Ax = b$. This method converges if $K^{-1}A$ has all its eigenvalues in the right half plane [15].

In [16,18] we study the effects of preconditioning on the Chebyshev Iteration method, when applied to linear sytems that arise from discretisation by finite differences of the p.d.e.

$$-(au'_x)'_x - (bu'_y)'_y + du'_x + eu'_y + cu = f ,$$

over a rectangular domain in R^2, with Dirichlet boundary conditions and with $a(x,y) > 0$, $b(x,y) > 0$, $c(x,y) \geq 0$.

Different preconditionings K^{-1} are considered, most of them are based upon incomplete decomposition of A. For some typical examples it is shown that the latter type of preconditioning leads to a highly competitive iterative method as compared to a number of other methods. For many relevant situations we are able to prove that $K^{-1}A$ has all its eigenvalues in the right half plane.

Special problems may be encountered when the coefficients $d(x,y)$ or $e(x,y)$ in the p.d.e. assume large values. It then often appears that the factors L and U of the incomplete decomposition are very ill-conditioned, whereas A is fairly well-conditioned. In [16,17,3 : chapter 4] we show how the ill-conditioning of the factors can be remedied by certain modifications of the incomplete decomposition algorithm. These modifications involve either a single parameter σ or simply replace the diagonal elements of L and U by values that guarantee well-conditioning.

We can prove that for a class of problems there are values of σ_0 (depending on the operator), such that $K^{-1}A$ has all its eigenvalues in the right half plane for $\sigma \geq \sigma_0$. An unsolved problem remains the experimental observation that the smallest value of σ which gives well-conditioned factors is also optimal with respect to the speed of convergence.

Analogously to the preconditioned cg method (see section 2) the complex Chebyshev Iteration method can be formulated in such a way that for the most relevant preconditionings, the preconditioned iterations require only little more computer time than the unpreconditioned iterations (see [16]).

Variants of the incomplete decomposition preconditionings that admit full vectorization on vector/parallel processors, can be easily constructed as is shown in [10,11].

Software for the preconditioned complex Chebyshev Iteration method is available in the program library ACCULIB [13].

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